Sigma master tape, a multi-group cross section library

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SIGMA MASTER TAPE, a Multi-Group Cross Section Library

by

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Abstract

The SIGMA MASTER TAPE is a cross section library for use in reactor physics calculations. It is generated from the UK Nuclear Data Library by the program SIGMA and contains the materials available in the UK Library, version 1968. The cross sections are given in a 76-group structure. The method of calculation and the contents of the tape are described together with the format and the use on the Borroughs B6700 computer.

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1. INTRODUCTION

Detailed nuclear data for reactor physics calculations are available in the form of evaluated libraries which are updated at intervals. The three main libraries, all of which are stored on magnetic tape in a form suitable for computer processing, are the ENDF/B[1], the KEDAK[2] and the UKNDL 3 and 4[3]. The present work is based on the UKNDL. By means of the processing program SIGMA the detailed data from the library are transformed into group cross sections. This, however, is a time-consuming calculation, and it was therefore decided to produce the group cross sections for relevant materials in a proper group structure once and store them on a magnetic tape which would then be the normal starting point for neutronics calculations. The SIGMA MASTER TAPE is the outcome of this procedure.

2. THE UKAEA NUCLEAR DATA LIBRARY

To produce the SIGMA MASTER TAPE the UKAEA Nuclear Data Library, version 1968, was used. The materials available in this version are listed in ref. 3. An updated library has been released in 1970, but as most of the modifications and additions are of minor importance for our use, it was not considered worthwhile to change to the new version. The contents of the 1970 version are listed in ref. 5.

2.1. Contents of the UKNDL

The UKNDL comprises data for most of the materials normally needed for reactor physics calculations. The library is subdivided into five files the contents of which can be outlined as follows:

File 1: U^{235}, U^{233}, Pu^{239}, U^{238} + the main moderating materials

File 2: The remaining heavy nuclides + the main structural materials + the poison materials B, Cd, and Xe

File 3: Some more rarely used materials, for instance materials of interest in experiments

File 4: Photon cross section data file

File 5: Capture cross sections for 78 fission products.

A data set in the library is identified by its "data file number", DFN. The DFN belongs to a substance (nuclide, natural element, molecule, or

mixture), and different data sets for the same substance are given different DFN's.

2.2. Data Representation in the UKNDL

For each substance the library may contain data for a number of reactions. Every reaction is identified by the reaction type number, RTN, which is subdivided into a "General classification number", GCN, and a "Particular classification number", PCN. The general classification numbers of interest here are the following:

1: Neutron cross section

2: Angular distribution of secondary neutrons

3: Energy distribution of secondary neutrons

4: $\bar{\nu}$ = mean number of secondary neutrons per fission

7: Thermal neutron scattering law data.

The PCN's used in the present library are given in table 2. The reaction type number of a given reaction is formed by combining the GCN and the PCN as follows:

$$RTN = 1000 \times GCN + PCN$$

Example: Angular distribution of neutrons from a (n, 2n) reaction has RTN 2016.

Data with GCN's 1 or 4 (cross sections, $\bar{\nu}$) are tabulated pointwise as a function of energy, the tables consisting of pairs of corresponding values of energy (MeV) and cross sections (barns) or $\bar{\nu}$. The energy points are spaced closely enough to ensure that interpolation in a log-log scale will give sufficient accuracy for all energies.

GCN 2 (angular distributions) are given as linear combinations of the probabilities of scattering as a function of $\cos\theta$, where θ is the scattering angle in either the centre of mass or the laboratory system. Linear interpolation is used between the $\cos\theta$-values. Angular distributions may be specified for either energy points or energy ranges. If pointwise representation is used, the distributions for energies in between the points are obtained by linear interpolation.

Energy distributions of secondary neutrons, GCN 3, are specified in the form of energy laws. The laws most often used are:

Table 2

List of PCN's used in the UKNDL, version 1968

1	Total
2	Elastic
3	Non-elastic = total minus elastic
4	(n, n') = total inelastic scattering summed over all final states
5-14	(n, n') to different levels
15	(n, n') to continuum
16	(n, 2n)
17	(n, 3n)
18	fission
22	(n, n') α
23	(n, n') 3α
24	(n, 2n) α
25	(n, 3n) α
26	(n, 2n) isomeric state
31-50	(n, n') to different levels
101	total parasitic absorption (no secondary neutrons)
102	(n, γ)
103	(n, p)
104	(n, d)
105	(n, t)
106	(n, He^3)
107	(n, α)
108	(n, 2α)

(1) neutrons emitted with energy $k(E_o - E_d)$, where k is a constant, E_o the initial energy, and E_d a constant energy (corresponding to inelastic scattering to a discrete level),

(2) pointwise tabulated spectrum of secondary neutron energies $p(E) = f(E)$ independent of initial neutron energy (used for instance for fission spectra),

(3) or dependent on initial energy E_o according to the formula $p\left(\frac{E}{E_o^q}\right) = f\left(E_o, \frac{E}{E_o^q}\right)$, where q may be 0, $\frac{1}{2}$, or 1.

In the case of tabulated probability distributions linear interpolation is used between the points.

Thermal scattering, GCN 7, is in the present version of the UKNDL only available for one material, C, and is therefore not included in the processing code SIGMA.

The data formats are described in more detail in ref. 4.

2.3. Use of Library Tapes on the B6700

At the Borroughs B6700 installation of Risø the following UKNDL files with corresponding file names are available:

File 1: AEK 105

File 2: AEK 122

File 3: AEK 121

File 5: AEK 120

The data are filed in EBCDIC card images on 9-track tapes, 800 BPI. The files are written with the file attributes KIND = 14, MAXRECSIZE = 14, BLOCKSIZE = 280. A list of the materials and processes on the four files is given in Appendix III.

3. THE SIGMA PROCESSING PROGRAM

The processing program SIGMA generates spectrum-averaged multigroup cross sections and transfer matrices from the pointwise tabulated data on the UKNDL. SIGMA is written in ILLINOIS-ALGOL for the IBM7094 machine, but has recently been transferred to the Borroughs B6700. The program is as yet only described in a preliminary internal report[6], but is very similar to the UK program GALAXY[7]. The function of SIGMA will be briefly described in the following.

3.1. Input Needed for a SIGMA Calculation

SIGMA uses as input the UKNDL file containing data for the materials to be processed. The user specifies the materials and the PCN's for each material and also provides the energy group structure to be used. The spectrum or weighting function over which the cross sections are to be averaged must be given as input, and it may be one of or a linear combination of four standard weighting functions:

(1) $F(E) = E^{-x}$ where x is a constant. If $x = 1$, this weighting function corresponds to the 1/E-flux.

(2) $F(E) = \frac{1}{(kT)^2} E \cdot \exp(-E/kT)$. This is the Maxwell spectrum, the value of kT must be specified.

(3) $F(E) = \frac{1}{E[1+(4.95 \cdot kT/E)^7]}$. The value of kT must be specified. This function is the Westcott delta 2 function, and it may be used to create a smooth joining between the Maxwell and the 1/E-spectrum.

(4) A tabulated weighting function, given as a number of energy points and corresponding spectrum values. Between the points the program performs log-log interpolation.

3.2. Quantities Computed by the Program

For all reactions (PCN's) the program computes the group average cross section in each group:

$$\phi_g = \frac{\int_g \phi(E)\, F(E)\, dE}{\int_g F(E)\, dE}$$

For all reactions resulting in the formation of secondary neutrons the Legendre moments of the group-to-group transfer matrix will be calculated:

$$\sigma^l_{g'g} = \frac{1}{\int_g F(E)\, dE} \int_{g'} dE' \int_g \sigma(E)\, F(E)\, dE \int_{-1}^{1} P_l(\mu)\, \Gamma(E, E', \mu)\, d\mu$$

A is the atomic weight.

This cross section is given PCN 205. It is not to be confused with the transport cross section, PCN 201, described in chapter 4.

Apart from the group cross sections the program calculates a number of material-independent quantities, i. e. quantities only dependent on the group structure and weighting spectrum used. These quantities are:

Group widths in energy

Group widths in lethargy

Group fluxes or normalizing factors, $\int_g F(E)\,dE$

Mean reciprocal velocities, $\dfrac{\int_g \frac{1}{v} F(E)\,dE}{\int_g F(E)\,dE}$

Mean energies, $\dfrac{\int_g E\,F(E)\,dE}{\int_g F(E)\,dE}$

Energy corresponding to the mean lethargy, $\exp\left(\dfrac{\int_g \ln E\,F(E)\,dE}{\int_g F(E)\,dE}\right)$

Proportion of the standard fission spectrum falling within the groups,

$$0.4527 \int_g \exp\left(-\frac{E}{0.965}\right) \sinh\sqrt{2.29\,E}\;dE$$

An outprint of the material-independent quantities (except the energy widths) calculated by SIGMA is shown in Appendix I.

SIGMA cannot handle all sorts of tabulated information which may be given in the UK-format. Thermal scattering, GCN 7, is not programmed into SIGMA, so when upscattering is important, the data must be supplied from other sources. In the UK-format options exist for tabulating of resolved and unresolved resonance parameters, but in the present version no

tables of this kind are found, and SIGMA cannot process them. GCN 3, energy distributions of secondary neutrons, may be given with a number of energy laws specified; two of them, laws 7 and 10, are not included in SIGMA. Law 7 (ref. 4) is not found in the 1968 version of the UKNDL, law 10 (ref. 3), however, is used once in DFN 328, tantalum.

4. STANDARD COMBINATION

For each material the UKNDL contains data for a number of reactions, characterized by the PCN's mentioned in section 2.2. A SIGMA run for a given material therefore produces cross sections and the required number of scattering matrices for, in some cases, a very great number of reactions. This is not desirable for practical use as neutronics codes normally do not distinguish between, for instance, elastic scattering and inelastic scattering to different levels. The Legendre expansion of scattering matrices will only be utilized in special programs as transport codes used for reference calculations, and most of the everyday codes can only account for scattering anisotropy by a transport correction to the cross sections. So it was decided to edit the group cross sections on the SIGMA MASTER TAPE in a standard combination which is supposed to be convenient for most of the applications.

The standard combination gives for each material the following combined cross sections with corresponding PCN's:

PCN 502, scattering cross section
+ transport-corrected scattering matrix

PCN 101, capture cross section

PCN 518, fission cross section
+ fission matrix

PCN 201, transport cross section.

The scattering cross section, PCN 502, is the sum of the cross sections for all scattering reactions, i.e. PCN 2, PCN 4 or PCN's 5-15 and PCN's 31-50. The processes (n, n') α and (n, n') 3α, PCN's 22 and 23, will, if they are met for a material, be added to the scattering cross section. The scattering matrix is transport-corrected, whereas the cross section is the total scattering cross section without any correction. The reason for this is that it allows the user of the data to calculate the magnitude of the employed

transport correction by subtracting the sum of the matrix columns from the group cross sections.

The capture cross section, PCN 101, is, if a total parasitic absorption cross section is given for a material, merely the group-averaged cross section for this process, PCN 101. Otherwise it is calculated as the sum of the cross sections for all processes which do not produce secondary neutrons, i.e. PCN's 102-108.

PCN 518, the fission cross section, comprises in addition to PCN 18, fission, all the processes that produce two or more neutrons, PCN's 16, 17, and 24-26. These neutron-multiplicating processes might have been regarded as a sort of inelastic scattering and added to the scattering cross section, but this would in some codes cause difficulties in conserving neutron balance. Their inclusion in the fission cross section has made it necessary to keep the full transfer matrix instead of representing the production of neutrons in the usual way by a fission spectrum and a mean $\bar{\nu}\sigma_f$ for each group because their secondary neutrons do not emerge with a spectrum independent of the energy of the primary neutron. The full matrix allows representation of an energy-dependent fission spectrum as well, but this has not been of interest with the present version of the UKNDL.

For use in the great number of neutronics codes which only accept a multiplication cross section $\bar{\nu}\sigma_f$ and a fission spectrum χ it is very easy to split the fission matrix into these two commonly used quantities. $\bar{\nu}\sigma_f$ in all groups is first obtained by summing the columns of the fission matrix:

$$\bar{\nu}\sigma_f^i = \sum_{j=1}^{G} FM^{ji}$$

where $\bar{\nu}\sigma_f^i$ is the cross section in group i, G is the number of groups, and FM^{ji} is the transfer cross section from group i to group j. After that an average fission spectrum is calculated by taking the mean value of the scattering into each group from all other groups. The fraction of the fission spectrum falling in group i will then be:

$$\chi^i = \frac{1}{G} \sum_j FM^{ij} / \bar{\nu}\sigma_f^j$$

In the usual case, where the main contribution to the fission matrix comes from a real fission process, this will be a good approximation.

The transport cross section, PCN 201, is the total cross section minus the transport correction. The total cross section in each group is found by adding the cross sections for PCN's 502, 101, and 518, and the transport cross section is therefore directly flux-weighted like the other cross sections and not inversely averaged as the transport cross section assigned PCN 205.

The transport correction applied is the usual correction suggested by Honeck (ref. 8). For the elastic scattering transfer matrix it is:

$$\sigma_{tr}^{ij} = \sigma_{o}^{ij} - \delta_{ij} \sum_{i=1}^{G} \sigma_{1}^{ij}$$

where σ_{o}^{ij} is the zeroth and σ_{1}^{ij} is the first Legendre moment of the transfer matrix. This correction leaves the off-diagonal elements and thus the energy transfer characteristics unaltered. The transport cross section in group j is obtained from the total cross section correspondingly:

$$\sigma_{tr}^{j} = \sigma_{total}^{j} - \sum_{i=1}^{G} \sigma_{1}^{ij}$$

To the inelastic part of the scattering no correction for anisotropy is made, because the transport correction of Honeck over-corrects the cross sections when neutrons are scattered from high-energy groups directly into groups of low energy. This is discussed in ref. 9.

5. GROUP STRUCTURE

It was the intention that the SIGMA MASTER TAPE should be adequate for use on a wide range of reactor types. This means that the energy groups applied must be sufficiently narrow to ensure that the group cross sections will be reasonably independent of the weighting spectrum used in SIGMA. On the other hand the number of energy groups is limited by practical considerations, as it ought to be possible to perform a spectrum calculation for at least a 3-region cell in the MASTER TAPE group structure.

At Risø the previous multi-group library has been that of LASER with its 85-group structure as described in ref. 10. About 85 groups was thought to be a realistic maximum considering the size of available computers. For the sake of continuity the LASER 85-group structure was chosen as the

starting point, and after the introduction of some modifications the result was a structure with 76 groups. These 76 energy groups are shown in Appendix I as an outprint from the SIGMA program.

The thermal energy mesh was taken over directly from LASER. It consists of 35 groups between 0 and 1.855 eV. Above the upper limit of the thermal mesh upscattering is assumed to be negligible. As seen from table 5 the group limits are round numbers in speed units of 2200 m/s which of course implies that the corresponding group energy boundaries and the lethargy widths have rather awkward values. A number of very narrow groups are placed around the Pu^{240} resonance at 1.0 eV, and the Pu^{239} resonance at 0.3 eV is treated similarly, but it is given fewer groups as it is low and broad compared with the sharp resonance of Pu^{240}. By means of these narrow groups the self-shielding of the two resonances is supposed to be accounted for, at least approximately, during Pu build-up, so that one set of microscopic group cross sections may be used for all geometries throughout depletion.

Apart from the two concentrations around the resonances, the thermal energy mesh is nearly equidistant in lethargy from about 0.05 eV and upwards where the thermal flux peak of an undermoderated light-water reactor is situated; downwards the groups get broader.

The fast and epithermal energy mesh of LASER is the well-known MUFT mesh starting from 10 MeV and stepping down in 0.25 lethargy unit steps until 67 keV. From here until 0.167 keV the lethargy widths are 0.5, and the rest of the way down to the thermal mesh it is again 0.25.

The fast part of the MUFT group structure is kept unaltered apart from one extra group which is added from 10 to 15 MeV. The reason for this is that the UKNDL contains data for energies up to 15 MeV.

In the resonance energy region it is of no use to try to make the groups narrow enough to represent the strongly energy-varying cross sections adequately. This would require thousands of groups. Instead one has to calculate the resonance broad group cross sections separately for each case, and they will be dependent both on geometry and on temperature. It is, however, possible to facilitate the resonance calculation by proper selection of the group boundaries.

First of all care should be taken to ensure that no important resonance is cut in two by a group boundary. But if the resonances in a group are either many uniformly distributed or one single resonance situated near the lethargy midpoint, it is in addition true to a good approximation that the group absorption cross section is independent of the source depletion through

Table 5

LASER thermal energy mesh

i	Speed[a] v_i	Mesh width[a] Δv_i	Energy E_i(ev)	E_{int}(ev)
1	.2	.2	.001012	.002277
2	.4	.2	.004048	.006325
3	.6	.2	.009108	.012397
4	.8	.2	.016192	.020493
5	1.0	.2	.0253	.030613
6	1.2	.2	.036432	.042757
7	1.4	.2	.049588	.056925
8	1.65	.3	.068879	.081972
9	1.95	.3	.096203	.11157
10	2.25	.3	.12808	.14573
11	2.55	.3	.16451	.18444
12	2.85	.3	.20550	.22770
13	3.075	.15	.23923	.25104
14	3.21	.12	.26069	.27053
15	3.33	.12	.28055	.29075
16	3.42	.06	.29592	.30113
17	3.505	.11	.31081	.32064
18	3.66	.2	.33891	.35768
19	3.91	.3	.38679	.41704
20	4.26	.4	.45913	.50326
21	4.715	.51	.56245	.62493
22	5.265	.59	.70132	.78211
23	5.845	.57	.86435	.95070
24	6.23	.2	.98197	1.01374
25	6.375	.09	1.02821	1.04277
26	6.435	.03	1.04765	1.05254
27	6.465	.03	1.05744	1.06236
28	6.495	.03	1.06728	1.07222
29	6.55	.08	1.08543	1.09873
30	6.69	.2	1.13233	1.16645
31	6.99	.4	1.23616	1.30791
32	7.39	.4	1.38169	1.45748
33	7.765	.35	1.52547	1.59500
34	8.10	.32	1.65993	1.72616
35	8.41135	.3027	1.79000	1.85500

[a] 1 unit = 2200 m/s

the group as shown by Askew in ref. 11. This will make it possible to calculate the resonance group cross sections on the basis of one single tabulation for each material.

In the LASER energy structure some of the group boundaries lie very close to important resonances. For that reason a number of group boundaries have been removed in the energy region from 1.855 eV up to 200 eV so that 18 groups are collapsed into only 8 groups. The main single resonances became situated near the middle of the lethargy interval of these broad groups.

In fig. 5 a, b, and c the resulting 76-group structure is shown. The original LASER structure is shown too for comparison. A light-water reactor spectrum was drawn to illustrate how the groups are concentrated round the fission spectrum at high energies and at the thermal part of the spectrum where also the two concentrations of very narrow groups are situated. In addition the energies of the low-lying U^{238} resonances are marked.

Although this group structure was designed mainly with reference to light-water reactors, it is hoped that it will be adequate for other reactor types as well. The 69-group structure used in WIMS (ref. 12) and in FLEF (ref. 13) is constructed according to similar principles and has been in use for both heavy-water- and graphite-moderated reactors. A group set commonly used for calculations on fast systems, the Bondarenko set (ref. 14), is included in fig. 5 showing that the fast part of the Risø 76-group system will presumably be suitable for fast reactor calculations.

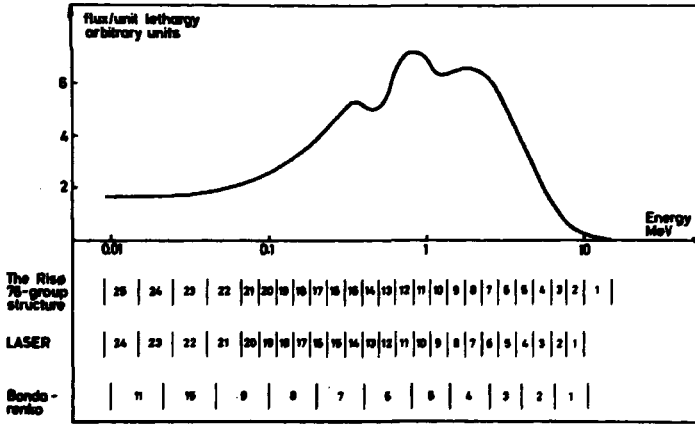

Fig. 5a. Energy groups. Fast part.

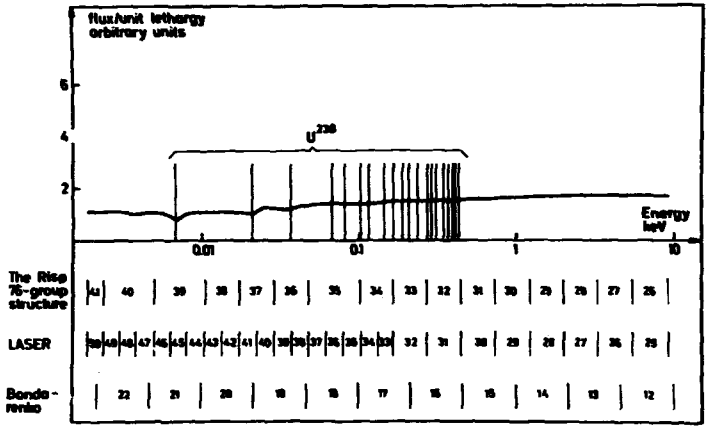

Fig. 5b. Energy groups. Intermediate part.

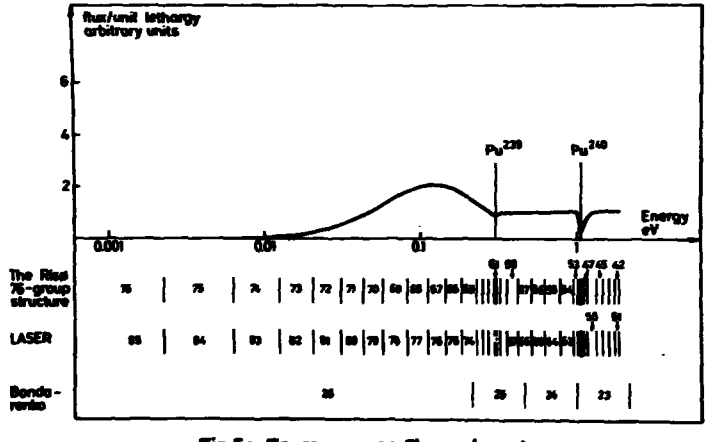

Fig. 5c. Energy groups. Thermal part.

6. WEIGHTING FUNCTION

Before the weighting function to be used for the SIGMA MASTER TAPE was chosen, a number of test runs were made where different weighting functions were used to generate cross sections for a number of materials in the 76-group structure decided upon. In resonance regions the group cross sections of course proved to be very spectrum-dependent, but where no resonances were present the most diverging weighting spectra gave a difference in the group cross section of only a few per cent. The conclusion drawn from this is that the groups of the 76-group structure are sufficiently narrow for a cross section tape intended for use on reactors with differing spectra.

As the weighting function seemed to be rather uncritical as long as it was not strongly inclined to the wrong side, a very simple combination of the standard weight functions available in SIGMA was chosen for the SIGMA MASTER TAPE. At low energies a Maxwell spectrum was used:

$$F(E) = \frac{1}{(kT)^2} \, E \cdot \exp\left(-\frac{E}{kT}\right)$$

with

$kT = 0.05$ eV

For all other energies the weighting function is simply

$$F(E) = \frac{1}{E}$$

The change from Maxwell to $\frac{1}{E}$ weighting was put between groups Nos. 63 and 64, i.e. at the energy 0.25 eV.

In resonance regions this weighting yields group cross sections for infinite dilution at the UKNDL temperature which is 300 degrees absolute.

7. UTILIZATION OF THE MASTER TAPE DATA IN THE PROGRAM SYSTEM AT RISØ

The SIGMA MASTER TAPE is one link in an attempt to build up a data generating system which produces constants for reactor physics calculations on the basis of fundamental nuclear data exclusively. Before the group cross sections are used in neutronics programs, they have to be supplied with thermal scattering data if the system in question is a thermal one, and with shielded resonance cross sections whenever the resonance absorbers may not be considered as infinitely dilute. This combination is performed in a program called CRS. After the cross sections for a given reactor configuration have been prepared, the code can make a spectrum calculation, collapse the cross sections into fewer groups, and punch the collapsed cross sections out in formats corresponding to the input requirements for a number of codes.

The thermal transfer cross sections are at present produced by a routine, NELKINSCM, which is incorporated in CRS. NELKINSCM (ref. 15) calculates thermal scattering matrices for H bound in H_2O and D in D_2O on the basis of the NELKIN model for H and the similar model for D. All other materials are treated as perfectly gaseous. In the near future this direct calculation of thermal scattering matrices is to be replaced by a thermal "master tape", where the transfer matrices will be filed for relevant materials at a number of temperatures close enough to allow linear interpolation between group cross sections in temperature. By the introduction of these tabulations much computer time will be saved, and at the same time the accuracy of the cross sections will be better as it is of course possible in the preparation of such tables to use more sophisticated methods than in a calculation which has to be made for every single case.

Effective resonance cross sections are introduced for U^{238} in 22 groups and for U^{235} and Pu^{239} in 14 groups. In both cases the lowest resonance group is the one just above the thermal upper limit, which means that the resonance region is defined to be 1.855 eV - 111 keV for U^{238} and 1.855 eV - 3.35 keV for U^{235} and Pu^{239}. The resonance cross sections may be calculated by the RESAB PROGRAM SYSTEM (refs. 16 and 17) or in the CRS program itself by the routine RESOREX (ref. 18) which generates resonance group cross sections by means of an equivalence principle on the basis of tabulations from RESAB. For all other resonant materials the dilute cross sections from the SIGMA MASTER TAPE are normally kept unaltered. In cases where shielding effects are considered important, the cross sections

may, however, be calculated by RESAB and substituted into the data set by hand.

For burn-up calculations a 10-energy group subsystem of the 76 MASTER TAPE groups is normally used in the burn-up codes CEB and CDB (ref. 19) in current use at Risø. As the 76-group spectrum changes because of build-up of Pu and fission products, it is advisable to regenerate the 10-group cross sections with revised isotopic composition at intervals during burn-up. If RESOREX is used, it is furthermore important to generate the Pu^{239} cross sections for a composition where a reasonable amount of Pu^{239} is present as demonstrated in ref. 18.

Frequent alternation between spectrum calculation in 76 groups and burn-up in 10 groups is possible for a pin cell burn-up calculation by the CEB program, but unrealistic in a box code like CDB. Fortunately it seems that 10-group cross sections generated by a spectrum calculated a few time steps from start may be used all through the burn-up calculation, giving an accuracy which is quite sufficient for most purposes.

8. CONTENTS OF THE CROSS SECTION LIBRARY

In its present version the SIGMA MASTER TAPE contains 126 materials which are almost all those available from the UKNDL, version 1968. For some materials only cross sections for a special reaction and in some cases for a limited energy range are given - these tables are not considered well suited for the standard combination described in chapter 4 and are therefore omitted. A single material was omitted because the SIGMA program at present cannot handle law number 10 for energy distribution of secondary neutrons which is used only in the tabulation for tatalum, DFN 328.

Each material on the SIGMA MASTER TAPE has an identification number which is to be used for seeking out the material. These numbers are written in order in one of the first records of the tape.

The cross sections are given in the standard combination which is described in chapter 4. In the combination all relevant detailed processes tabulated for each material are included. The UKNDL specifies data for detailed reactions by means of particular classification numbers, PCN's, as described in section 2.2. In Appendix III a listing is given of the reactions of the different materials.

8.1. Table of the Contents

In table 8.1 the SIGMA MASTER TAPE contents are listed. The materials are put in order of increasing mass number apart from the 78 fission products from UKNDL file 5 which are taken last. For each material the identification number is given, and the processes from the standard combination that are found for a particular material are given.

For most substances only one file on the UKNDL is available. In cases of doubt it is noted in the table which DFN has been used. Where an element is mentioned without mass number, the cross section set refers to the natural isotopic composition.

The pseudo-fission-product called FP is generated from DFN 106 in the UKNDL. Since no information is given about the reactor configuration to which it applies, great care should be taken in using it for reactor physics calculations. The large absorption cross section indicates that all fission products are included, i. e. also Xe and Sm.

8.2. Sequence of Materials

To minimize the computer time wasted on the reading of the magnetic tape, care was taken to place the materials so that those most often used are set first. In table 8.2 the materials are listed in the same sequence as on the tape.

8.3. Missing Materials and Energy Regions

A number of materials of interest in reactor physics calculations are not included in the UKNDL and are consequently not found on the SIGMA MASTER TAPE either. Such materials must, when necessary, be taken from other sources. For example Pu^{242}, Ag, and In are missing.

In some cases the cross sections of the UKNDL are only tabulated for a smaller energy range than the standard range from 10^{-4} eV to 15 MeV. In energy groups where no data exist the cross sections are set equal to zero, and the limited energy range is noted in table 8.1. For some of the materials, however, the data stop at 10 MeV so that the cross section in the first energy group is zero. This has not caused any comment in the table.

Table 8.1

Contents of the SIGMA MASTER TAPE

Material	Number	PCN's				Comments
		502 + matrix	101	518 + matrix	201	
H	41	x	x		x	
H_2O	34	x	x		x	Only for energies < 0.5 eV
D	42	x	x	x	x	
D_2O	33	x	x		x	Only for energies < 9 eV
T	61	x	x	x	x	
He^3	66	x	x		x	Temperature 0 K
He^4	67	x	x		x	Temperature 0 K
Li^6	68	x	x	x	x	
Li^7	69	x	x	x	x	Temperature 0 K
Be^9	40	x	x	x	x	
B	50	x	x		x	
B^{10}	64	x	x		x	
B^{11}	65	x	x		x	
C	32	x	x		x	
N	71	x	x	x	x	
O	31	x	x		x	DFN 34 has been used
F	70	x	x	x	x	
Na	46	x	x	x	x	DFN 182 has been used
Al	35	x	x	x	x	DFN 35 has been used
Si	63	x	x		x	
Cl	73	x	x	x	x	
Ca	72	x	x		x	
Ti	75	x	x	x	x	
Cr	38	x	x	x	x	
Mn^{55}	51		x			
Fe	37	x	x		x	
Ni	39	x	x	x	x	
Cu	53	x	x	x	x	
Ga	74	x	x	x	x	

Material	Number	PCN's				Comments
		502 + matrix	101	518 + matrix	201	
Zr	36	x	x	x	x	
Cd	49	x	x	x	x	
Xe^{135}	19	x	x		x	
Sm^{149}	15		x			Identical with fission product No. 767
Gd	76		x			Only for energies $\langle 3$ eV
W	57	x	x	x	x	
Au^{197}	58	x	x	x	x	
Pb	43	x	x	x	x	
Th^{232}	1	x	x	x	x	
U^{233}	3	x	x	x	x	
U^{234}	4	x	x	x	x	Only for energies $\rangle 1$ keV
U^{235}	5	x	x	x	x	
U^{236}	6	x	x	x	x	Only for energies $\rangle 1$ keV
U^{238}	7	x	x	x	x	
Pu^{238}	62	x	x	x	x	
Pu^{239}	9	x	x	x	x	
Pu^{240}	10	x	x	x	x	
Pu^{241}	11	x	x	x	x	
FP	28	x	x	x	x	Pseudo-fission-products
Br^{81}	701		x			
Se^{82}	702		x			
Kr^{83}	703		x			
Kr^{84}	704		x			
Kr^{85}	705		x			
Rb^{85}	706		x			
Kr^{86}	707		x			
Rb^{87}	708		x			
Sr^{88}	709		x			
Sr^{89}	710		x			
Y^{89}	711		x			

Material	Number	PCN's				Comments
		502 + matrix	101	518 + matrix	201	
Sr^{90}	712		x			
Y^{90}	713		x			
Y^{91}	714		x			
Zr^{91}	715		x			
Zr^{92}	716		x			
Zr^{93}	717		x			
Zr^{94}	718		x			
Mo^{95}	719		x			
Zr^{96}	720		x			
Mo^{97}	721		x			
Mo^{98}	722		x			
Tc^{99}	723		x			
Mo^{100}	724		x			
Ru^{101}	725		x			
Ru^{102}	726		x			
Rh^{103}	727		x			
Ru^{104}	728		x			
Rh^{105}	729		x			
Pd^{105}	730		x			
Pd^{106}	731		x			
Pd^{107}	732		x			
Pd^{108}	733		x			
Ag^{109}	734		x			
Cd^{113}	735		x			
In^{115}	736		x			
Sb^{125}	737		x			
I^{127}	738		x			
Te^{128}	739		x			
I^{129}	740		x			
Te^{130}	741		x			
I^{131}	742		x			
Xe^{131}	743		x			
Xe^{132}	744		x			
Xe^{133}	745		x			
Cs^{133}	746		x			

Material	Number	PCN's				Comments
		502 + matrix	101	518 + matrix	201	
Xe^{134}	747		x			
Cs^{134}	748		x			
I^{135}	749		x			
Xe^{135}	750		x			
Cs^{135}	751		x			
Xe^{136}	752		x			
Cs^{137}	753		x			
Ba^{138}	754		x			
La^{139}	755		x			
Ce^{140}	756		x			
Pr^{141}	757		x			
Ce^{142}	758		x			
Nd^{143}	759		x			
Nd^{144}	760		x			
Nd^{145}	761		x			
Nd^{146}	762		x			
Pm^{147}	763		x			
Nd^{148}	764		x			
Pm^{148}	765		x			
Pm^{146m}	766		x			
Sm^{149}	767		x			
Nd^{150}	768		x			
Sm^{150}	769		x			
Sm^{151}	770		x			
Sm^{152}	771		x			
Eu^{153}	772		x			
Sm^{154}	773		x			
Eu^{154}	774		x			
Eu^{155}	775		x			
Gd^{155}	776		x			
Gd^{156}	777		x			
Gd^{157}	778		x			

Table 8.2

Materials in order as filed on the tape

No.	Identification number	Material
1	5	U^{235}
2	7	U^{238}
3	41	H
4	42	D
5	31	O
6	32	C
7	34	H_2O
8	33	D_2O
9	40	Be^{9}
10	46	Na
11	36	Zr
12	37	Fe
13	38	Cr
14	39	Ni
15	35	Al
16	50	B
17	49	Cd
18	9	Pu^{239}
19	10	Pu^{240}
20	11	Pu^{241}
21	6	U^{236}
22	1	Th^{232}
23	3	U^{233}
24	4	U^{234}
25	19	Xe^{135}
26	28	FP
27	15	Sm^{149}
28	53	Cu
29	58	Au^{197}
30	57	W
31	43	Pb
32	51	Mn^{55}
33	61	T
34	62	Pu^{238}
35	63	Si
36	64	B^{10}
37	65	B^{11}
38	66	He^{3}
39	67	He^{4}
40	68	Li^{6}
41	69	Li^{7}
42	70	F
43	71	N
44	72	Ca
45	73	Cl
46	74	Ga
47	75	Ti
48	76	Gd
49	701	Br^{81}
50	702	Se^{82}
51	703	Kr^{83}
52	704	Kr^{84}
53	705	Kr^{85}
54	706	Rb^{85}
55	707	Kr^{86}
56	708	Rb^{87}
57	709	Sr^{88}
58	710	Sr^{89}
59	711	Y^{89}
60	712	Sr^{90}
61	713	Y^{90}
62	714	Y^{91}
63	715	Zr^{91}
64	716	Zr^{92}
65	717	Zr^{93}
66	718	Zr^{94}
67	719	Mo^{95}
68	720	Zr^{96}

No.	Identification number	Material
69	721	Mo^{97}
70	722	Mo^{98}
71	723	Tc^{99}
72	724	Mo^{100}
73	725	Ru^{101}
74	726	Ru^{102}
75	727	Rh^{103}
76	728	Ru^{104}
77	729	Rh^{105}
78	730	Pd^{105}
79	731	Pd^{106}
80	732	Pd^{107}
81	733	Pd^{108}
82	734	Ag^{109}
83	735	Cd^{113}
84	736	In^{115}
85	737	Sb^{125}
86	738	I^{127}
87	739	Te^{128}
88	740	I^{129}
89	741	Te^{130}
90	742	I^{131}
91	743	Xe^{131}
92	744	Xe^{132}
93	745	Xe^{133}
94	746	Cs^{133}
95	747	Xe^{134}
96	748	Cs^{134}
97	749	I^{135}
98	750	Xe^{135}
99	751	Cs^{135}
100	752	Xe^{136}
101	753	Cs^{137}
102	754	Ba^{138}
103	755	La^{139}

No.	Identification number	Material
104	756	Ce^{140}
105	757	Pr^{141}
106	758	Ce^{142}
107	759	Nd^{143}
108	760	Nd^{144}
109	761	Nd^{145}
110	762	Nd^{146}
111	763	Pm^{147}
112	764	Nd^{148}
113	765	Pm^{148}
114	766	Pm^{148m}
115	767	Sm^{149}
116	768	Nd^{150}
117	769	Sm^{150}
118	770	Sm^{151}
119	771	Sm^{152}
120	772	Eu^{153}
121	773	Sm^{154}
122	774	Eu^{154}
123	775	Eu^{155}
124	776	Gd^{155}
125	777	Gd^{156}
126	778	Gd^{157}

9. MAGNETIC TAPE STRUCTURE

9.1. Format of the Binary Tape

In deciding upon the format of the binary tape the philosophy was that of making the tape easy to read by user programs rather than that of saving magnetic tape space. One result of this is that the full scattering matrices were recorded, although in some cases they mostly consist of noughts.

In the following the contents of the binary tape are listed record by record. All arrays running over energy groups start in group 1 which is the group of highest energy.

(a) 4 Words:

SET, integer	= set number of the data on the tape, refers to the group structure and weighting function used. The present version has set number 1
GRP, integer	= number of energy groups
MAT, integer	= number of materials
LEG, integer	= maximal order of Legendre moments for scattering matrices which is 0 for the standard combination used on the SIGMA MASTER TAPE

(b) 8 x GRP + MAT + 1 Words (nine physical records, one for each array):

E [0:GRP], real array	= energy group boundaries (MeV)
DE [1:GRP], real array	= group energy widths (MeV)
DU [1:GRP], real array	= group lethargy widths
NORM [1:GRP], real array	= group normalizing factors
EMEAN [1:GRP], real array	= weighted group mean energies (MeV)
EUMEAN [1:GRP], real array	= energies corresponding to the weighted group mean lethargies (MeV)
VRECMEAN [1:GRP], real array	= group mean reciprocal velocities(s/cm)
FISP [1:GRP], real array	= fraction of the standard fission spectrum falling within each group
NUMB [1:MAT], integer array	= identification numbers of the materials on the tape

The following is repeated for all materials, i. e. MAT times

(c) 6 Words:

DFN, integer	= data file number from the UKNDL for the material
AW, real	= atomic weight (amu)
Z, integer	= atomic number
TXT	= alphanumeric name of the material (6 characters)
NPCA, integer	= number of PCN's given for this material (NPCA is 1, 3, or 4 on the SIGMA MASTER TAPE)
N, integer	= identification number of the material. This number is one of the elements of the NUMB array in record b.

(d) 2 x NPCA Words:

PCN [1:NPCA], integer array	= particular classification numbers for the NPCA different cross section types of the material
MIND [1:NPCA], integer array	= matrix indicators. An element of the MIND array is 1 if the corresponding cross section is followed by a scattering matrix, if not, it is -1.

The following records, type e and, if the MIND-element is 1, GRP times type f, are repeated NPCA times, i. e. once for each cross section type of the material.

(e) GRP Words:

SIG [1:GRP], real array	= group cross sections

(f) GRP Words:

SM [I, 1:GRP], real array	= transfer cross section to group I from all other groups

Record f is repeated GRP times, I running from 1 to GRP, to give the full scattering matrix.

After the last material an END-OF-FILE mark is written.

9.2. Characteristics of the Tape Version for Use on the B6700

The SIGMA MASTER TAPE in use on the Borroughs B6700 computer at Risø is a 9-track 800 BPI binary tape. It is written with the file attribute FILETYPE = 0 which means constant physical record length equal to the value of the file attribute MAXRECSIZE. The records are unblocked. Two versions of the SIGMA MASTER TAPE exist at present:

A 2400-feet tape labelled AEK134 containing all 126 materials. This version is filed with MAXRECSIZE = 126.

A 1200-feet tape labelled AEK42 which contains only the first 32 materials. It has MAXRECSIZE = 77.

In case the binary tape is spoiled, for instance by a parity error, it may be regenerated from a card image version by use of a small program called MTBIN. This is described in Appendix II.

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REFERENCES

1) Data Formats and Procedures for the ENDF Neutron Cross Section Library. Edited by M.K. Drake. BNL 50274 (1970) 200 pp.

2) D. Woll, Card Image Format of the Karlsruhe Evaluated Nuclear Data File KEDAK. KFK 880 (1968) 18 pp.

3) D.S. Norton, The UKAEA Nuclear Data Library, February 1968. AEEW-M 824 (1968) 23 pp.

4) K. Parker, The Aldermaston Nuclear Data Library as at May 1983. AWRE O-70/63 (1963) 64 pp.

5) A Compilation of Evaluations of Neutron Cross Sections Available at October 1970. CCDN-NW/12 (1970).

6) J. Pedersen, A Preliminary Description of the SIGMA Programme. Risø-M-949 (1969) (Internal Report) 29 pp.

7) V.J. Bell et al., A User's Guide to GALAXY 3. AEEW-R-379 (1964) 58 pp.

8) H.C. Honeck, The Calculation of the Thermal Utilization and Disadvantage Factor in Uranium/Water Lattices. Nucl. Sci. Eng. 18 (1964) 49-68.

9) H. Neltrup, Integral Transport Theory in Various Geometries. Risø-M-1289 (1970) 13 pp.

10) C.G. Poncelet, LASER - A Depletion Program for Lattice Calculations based on MUFT and THERMOS. WCAP-6073 (1966) 104 pp.

11) J.R. Askew, The Calculation of Resonance Captures in a Few-Group Approximation. AEEW-R-489 (1966) 22 pp.

12) J.R. Askew, F.J. Fayers, and P.B. Kemshell, A General Description of the Lattice Code WIMS. J. Brit. Nucl. Energy Soc. 5, (1966) 564-585.

13) I. Carlvik, Methods and Computer Codes Developed in Sweden for Reactor Physics Calculations, Tekniska Högskolan, Avd. för Teknisk Fysik, Finland. Rapport Nr. 506/1969 (in Swedish, 1969) 106 pp.

14) L.P. Abagjan et al., Gruppenkonstanten schneller und intermediärer Neutronen für die Berechnung von Kernreaktoren. KFK-tr-144 (in German) 212 pp.

15) C.F. Højerup, Risø, Denmark, unpublished work.

16) J. Mikkelsen, The Neutron Resonance Reactions in Thermal Nuclear Reactors Determined by Semi-Analytic as well as Numerical Methods. Risø Report No. 234 (1970) 167 pp.

17) J. Mikkelsen and P. Kirkegaard, A User's Guide to the RESAB Program System for the B6700 Computer. Risø-M-1477 (1972) 53 pp.

18) H. Neltrup, RESOREX, A Procedure for Calculating Resonance Group Cross-Sections. Risø-M-1437 (1971) 25 pp.

19) K.E. Lindstrøm Jensen, Development and Verification of Nuclear Calculation Methods for Light-Water Reactors. Risø Report No. 235 (1971) 161 pp.

APPENDIX I

OUTPRINT OF THE GROUP STRUCTURE FROM THE SIGMA PROGRAM

On the following pages the 76-group structure is shown as printed out by the SIGMA program. Apart from the energy boundaries the group structure is characterized by the lethargy widths of the groups and by the proportion of the standard fission spectrum belonging to each group (section 3.2). The quantities average energy, energy at average lethargy, and average inverse velocity are dependent on the weighting function specified, in this case the weighting function used for the SIGMA MASTER TAPE as described in chapter 6. The group constants called NORM in the table are the group fluxes, i.e. the weighting function integrated for each group.

GROUP NUMBER	ENERGY BOUNDARIES (MEV)	AVERAGE ENERGY (MEV)	ENERGY AT AVERAGE LETHARGY (MEV)	LETHARGY WIDTH	FRACTION OF STANDARD FISSION SPECTRUM	AVERAGE INVERSE VELOCITY (SEC/CM)	NORM
1.	1.9000E 01	1.2332E 01	1.2267E 01	4.0547E-01	0.00360	2.0697E-08	4.3547E-31
2.	1.0000E 01	6.0400E 00	6.0293E 00	2.5000E-01	0.00911	2.4356E-08	2.9.8.E-31
3.	7.7800E 00	6.0000E 00	6.0729E 00	2.5000E-01	0.01705	2.7509E-08	2.9054E-31
4.	6.0653E 00	5.3686E 00	5.3516E 00	2.5000E-01	0.03944	3.1274E-08	2.9006E-31
5.	4.7237E 00	4.1795E 00	4.1686E 00	2.5000E-01	0.06872	3.9433E-08	2.9008E-31
6.	3.6788E 00	3.2350E 00	3.2465E 00	2.5000E-01	0.09625	4.9156E-08	2.9003E-31
7.	2.8650E 00	2.5350E 00	2.5254E 00	2.5000E-01	0.11403	6.3503E-08	2.9005E-31
8.	2.2313E 00	1.9742E 00	1.9691E 00	2.5000E-01	0.11865	9.1962E-08	2.9006E-31
9.	1.7377E 00	1.5373E 00	1.5339E 00	2.5000E-01	0.11236	9.8421E-08	2.9003E-31
10.	1.3533E 00	1.1976E 00	1.1943E 00	2.5000E-01	0.09859	6.8207E-08	2.9003E-31
11.	1.0540E 00	9.3257E-01	9.3014E-01	2.5000E-01	0.08174	7.5822E-08	2.9006E-31
12.	8.2085E-01	7.2622E-01	7.2463E-01	2.5000E-01	0.06489	8.9011E-08	2.9003E-31
13.	6.3928E-01	5.6563E-01	5.6418E-01	2.5000E-01	0.04984	9.6330E-08	2.9005E-31
14.	4.9787E-01	4.4051E-01	4.3937E-01	2.5000E-01	0.03732	1.0916E-07	2.9006E-31
15.	3.8774E-01	3.4307E-01	3.4218E-01	2.5000E-01	0.02741	1.2346E-07	2.9006E-31
16.	3.0197E-01	2.6719E-01	2.6649E-01	2.5000E-01	0.01983	1.4016E-07	2.9003E-31
17.	2.3518E-01	2.0808E-01	2.0754E-01	2.5000E-01	0.01418	1.5882E-07	2.9003E-31
18.	1.8316E-01	1.6206E-01	1.6163E-01	2.5000E-01	0.01009	1.7997E-07	2.9001E-31
19.	1.4264E-01	1.2621E-01	1.2585E-01	2.5000E-01	0.00708	2.0393E-07	2.9003E-31
20.	1.1109E-01	9.8292E-02	9.8037E-02	2.5000E-01	0.00499	2.3108E-07	2.9006E-31
21.	8.6517E-02	7.6550E-02	7.6391E-02	2.5000E-01	0.00345	2.6196E-07	2.9003E-31
22.	6.7379E-02	5.9626E-02	5.9475E-02	5.0000E-01	0.00407	3.1647E-07	5.0003E-31
23.	4.0868E-02	3.2160E-02	3.1820E-02	5.0000E-01	0.00195	4.0636E-07	5.0000E-31
24.	2.4787E-02	1.9506E-02	1.9335E-02	5.0000E-01	0.00093	5.2177E-07	5.0003E-31
25.	1.5034E-02	1.1831E-02	1.1709E-02	5.0000E-01	0.00044	6.6997E-07	5.0003E-31
26.	9.1188E-03	7.1759E-03	7.1017E-03	5.0000E-01	0.00021	8.6026E-07	5.0003E-31
27.	5.5308E-03	4.3524E-03	4.3074E-03	5.0000E-01	0.00010	1.1044E-06	5.0000E-31
28.	3.3546E-03	2.6399E-03	2.6126E-03	5.0000E-01	0.00005	1.4183E-06	5.0000E-31
29.	2.0347E-03 1.2341E-03	1.6012E-03	1.5846E-03	5.0000E-01	0.00002	1.8212E-06	5.0000E-31

30.	7.40828E-04	9.71168-04	9.61118-04	5.00008-01	0.00001	2.33848-06	9.00008-31
31.	4.94008-04	5.89048-04	5.62958-04	5.00008-01	0.00000	3.00268-06	9.00008-31
32.	2.75368-04	3.57278-04	3.53988-04	5.00008-01	0.00000	3.85948-06	9.00008-31
33.	1.67028-04	2.16698-04	2.14658-04	5.00008-01	0.00000	4.95058-06	9.00838-31
34.	1.01308-04	1.31438-04	1.30278-04	5.00008-01	0.00000	6.33698-06	9.00038-31
35.	6.78518-05	7.12668-05	6.94238-05	7.50008-01	0.00000	8.71648-06	7.50008-31
36.	2.90238-05	3.76548-05	3.72678-05	5.00038-01	0.00000	1.18748-05	5.00038-31
37.	1.76028-05	2.28408-05	2.26038-05	5.00008-01	0.00000	1.52488-05	5.00008-31
38.	1.06778-05	1.38538-05	1.37138-05	5.00318-01	0.00000	1.95798-05	5.00318-31
39.	5.04358-06	7.31148-06	7.33828-06	7.50008-01	0.00000	2.68498-05	7.50008-31
40.	2.38248-06	3.54018-06	3.44638-06	7.50008-01	0.00000	3.90658-05	7.50008-31
41.	1.65508-06	2.10778-06	2.10228-06	2.50218-01	0.00000	4.99038-05	2.50218-31
42.	1.72628-06	1.78988-06	1.78948-06	7.19628-02	0.00000	5.40868-05	7.19628-32
43.	1.99308-06	1.65978-06	1.65938-06	7.98498-02	0.00000	5.61378-05	7.98498-32
44.	1.45758-06	1.52528-06	1.52478-06	9.01918-02	0.00000	5.85638-05	9.01918-32
45.	1.33708-06	1.36148-06	1.38078-06	1.08388-01	0.00000	6.19448-05	1.38308-31
46.	1.16648-06	1.23588-06	1.23518-06	1.14508-01	0.00000	6.50718-05	1.14508-31
47.	1.09878-06	1.13228-06	1.13238-06	9.97968-02	0.00000	6.79838-05	9.97968-32
48.	1.37228-06	1.08548-06	1.08538-06	2.44158-02	0.00000	6.94068-05	2.44158-32
49.	1.06248-06	1.06738-06	1.06768-06	9.18218-03	0.00000	6.99918-05	9.18218-33
50.	1.05258-06	1.05748-06	1.05768-06	9.36228-03	0.00000	7.03168-05	9.36228-33
51.	1.04268-06	1.04778-06	1.04778-06	9.25898-03	0.00000	7.06448-05	9.25898-33
52.	1.01378-06	1.02828-06	1.02818-06	2.83028-02	0.00000	7.13118-05	2.83028-32
53.	9.50708-07	9.81868-07	9.81718-07	6.41648-02	0.00000	7.24018-05	6.41648-32
54.	7.82118-07	8.63668-07	8.62298-07	1.09208-01	0.00000	7.78948-05	1.98208-31
55.	6.24938-07	7.00568-07	6.99128-07	2.24368-01	0.00000	8.69238-05	2.24368-31
56.	5.03268-07	5.61988-07	5.60818-07	2.16538-01	0.00000	9.66028-05	2.16538-31
57.	4.17048-07	4.58868-07	4.58128-07	1.87928-01	0.00000	1.06378-04	1.87928-31
58.	3.57688-07	3.86688-07	3.86228-07	1.53548-01	0.00000	1.16358-04	1.53548-31
59.	3.20648-07	3.38828-07	3.38658-07	1.30328-01	0.00000	1.24278-04	1.09328-31

60.	5.0113E-07	3.1878E-07	3.1873E-07	6.2777E-02	0.00000	1.2972E-04	6.2777E-02
61.	2.9975E-07	2.9991E-07	2.9990E-07	3.5979E-02	0.00000	1.3293E-04	3.5978E-02
62.	2.7059E-07	2.8052E-07	2.8044E-07	7.2081E-02	0.00000	1.3654E-04	7.2081E-02
63.	2.5104E-07	2.6066E-07	2.6063E-07	7.4771E-02	0.00000	1.4165E-04	7.4771E-02
64.	2.2770E-07	2.3865E-07	2.3864E-07	9.7583E-02	0.00000	1.4686E-04	1.0782E-01
65.	1.8444E-07	2.0373E-07	2.0336E-07	2.1070E-01	0.00000	1.4842E-04	9.8773E-02
66.	1.4573E-07	1.6336E-07	1.6298E-07	2.3957E-01	0.00000	1.7921E-04	9.9643E-02
67.	1.1137E-07	1.2767E-07	1.2709E-07	2.6710E-01	0.00000	2.0297E-04	1.3471E-01
68.	9.1972E-08	9.8695E-08	9.8695E-08	3.0827E-01	0.00000	2.3397E-04	1.6330E-01
69.	6.6925E-08	6.9162E-08	6.8785E-08	3.8444E-01	0.00000	2.7608E-04	1.7267E-01
70.	4.2797E-08	4.9843E-08	4.9675E-08	2.8629E-01	0.00000	3.2470E-04	1.0389E-01
71.	3.0613E-08	3.6776E-08	3.6608E-08	3.3411E-01	0.00000	3.7839E-04	8.5196E-02
72.	2.0493E-08	2.5718E-08	2.5551E-08	4.0134E-01	0.00000	4.5314E-04	6.1740E-02
73.	1.2397E-08	1.6670E-08	1.6504E-08	5.0263E-01	0.00000	5.6428E-04	3.8116E-02
74.	6.3290E-09	9.6297E-09	9.4675E-09	6.7294E-01	0.00000	7.4643E-04	1.8742E-02
75.	2.2770E-09	4.5951E-09	4.4399E-09	1.0217E 00	0.00000	1.0953E-03	6.3913E-03
76.	1.0000E-10	1.5146E-09	1.3824E-09	3.1254E 00	0.00000	2.0114E-03	1.0640E-03

APPENDIX II

CARD IMAGE VERSION OF THE SIGMA MASTER TAPE AND THE PROGRAM MTBIN FOR GENERATION OF THE BINARY TAPE

The SIGMA MASTER TAPE normally used is a binary tape for the Borroughs B6700 computer at Risø. Unfortunately a tape may now and then be spoiled by, for instance, a parity error, and it is therefore important to be able to regenerate it if necessary. The binary SIGMA MASTER TAPE is backed up by a card image version of the information which may also be used in transferring the library to another computer.

The card image version is filed on 3 magnetic tapes labelled AEK133, AEK108, and AEK110 and containing a total of 78,806 cards. The format of the card image version is the same as for the binary tape described in section 9.1, except that a "record" now means the number of cards necessary to hold the information from a binary record. On each card the information is printed in the first 72 columns, and the remaining 8 are used for numbering of the cards.

All cards are printed in the format 6E12.5 except for the card containing the first record of the tape which has the format 4F12.0, X24, and the first card for each new material which contains an alphanumeric variable and has therefore been given the format 3E12.5, X3, A6, X3, 2E12.5. Where a card is not fully utilized, the remaining places are filled up by noughts. In front of the tapes one card containing a heading is placed, and its text is

on AEK133: SIGMA MASTER TAPE PART 1

on AEK108: SIGMA MASTER TAPE PART 2

on AEK110: SIGMA MASTER TAPE PART 3

The card image tapes must be read with the file attributes

MAXRECSIZE = 14

BLOCKSIZE = 280

which means that the tapes are blocked with 20 cards in each block. The tapes are 9 track tapes in EBCDIC, written with the density 800BPI.

To generate the binary tape from the three EBCDIC tapes a small ALGOL-program, MTBIN, was written. The program has no card input,

so the only thing necessary to do before a run is that the binary output tape which is called FILMT internally in the program must be connected with the physical output tape. This is most easily done by inserting one card after the first BEGIN in the program with the text:

DEFINE FILMT = TAPENO ## ;

The name TAPENO must be declared as follows:

FILE TAPENO (KIND = 14, MAXRECSIZE = 126, SAVEFACTOR = 999);

TAPENO will then be the label of the binary tape produced.

APPENDIX III

MATERIALS AND PROCESSES IN THE UKNDL, VERSION 1968

In the following the contents of the UKNDL, version 1968, are listed. For each of the four files, files 1, 2, 3, and 5, the materials and processes are printed. A material is identified by its data file number, DFN, and described by the name following immediately after the DFN. The reactions given for each material are identified by the reaction type number of which the first digit is the general classification number, GCN, and the last three form the particular classification number, PCN, as explained in section 2.2.

For each reaction as well as for each material the number of records or cards is given.

CONTENTS OF GALAXY LIBRARY TAPE FILE NO 1

TOTAL 19050 RECORDS

DFN	MATERIAL	RECORDS	REACTION	RECORDS
67	H	292		
			1001	84
			1002	84
			2003	37
			1102	84
27	H20	39		
			1001	0
			1002	0
			2003	1
			1003	0
			1102	0
210	D	221		
			1001	20
			1002	20
			2003	06
			1003	20
			1016	10
			2016	9
			3016	37
			1102	20
26	D2U	103		
			1001	26
			1002	26
			2003	3
			1003	26
			1101	26
219	T	184		
			1001	26
			1002	26
			2003	93
			1003	10
			1016	10
			2016	3
			3016	13
50	BE9	361		
			1001	40
			1002	40
			2003	124
			1003	40
			1024	15
			2024	25
			3024	33
			1102	13
			1105	5
			1107	20
7	BE0	75		
			1001	17
			1002	17
			2003	3
			1003	17
			1101	17
51	C	2256		
			1001	121
			1002	121
			2003	958
			7002	651
			1061	121
34	O	1092		
			1001	136
			1002	136
			2003	203
			1003	136
			1004	31
			2004	3
			1005	36
			2005	3
			1006	31
			2006	3
			1007	20
			2007	3
			1008	19
			2008	3
			1009	12
			2000	1
			1010	11
			2010	3
			1011	10
			2011	3
			1012	9
			2012	3
			1013	7
			2013	3
			1014	7
			2014	3
			1031	6
			2031	3
			1032	6
			2032	3
			1033	5
			2033	3
			1034	5
			2034	3
			1035	5
			2035	3
			1036	4
			2036	3
			1037	4
			2037	3
			1038	4
			2038	3
			1039	4
			2039	3
			1040	3
			2040	3
			1041	3
			2041	3
			1042	3
			2042	3
			1102	4
			1103	10
			1104	10
			1107	81
66	U235	4134		
			1001	662
			1002	662
			2003	180
			1003	662
			1005	11
			2005	3
			1005	64
			2005	3
			1023	31
			2023	3
			3023	17
			1102	121

CONTENTS OF GALAXY LIBRARY TAPE FILE NO 8

TOTAL 19035 RECORDS

BPN	MATERIAL	RECORDS	REACTION	RECORDS
261	PU240	1055		
			1001	83
			1009	83
			2009	166
			1003	83
			1004	29
			2004	3
			1006	29
			2006	3
			1007	10
			2007	3
			1014	30
			2014	21
			3014	47
			1016	11
			2016	5
			3016	136
			1017	5
			2017	7
			3017	14
			101A	46
			201A	3
			301A	71
			401A	5
			1109	83
60	PU241	2155		
			1001	270
			1009	270
			2009	186
			1003	270
			1014	96
			2014	71
			3014	38
			1016	9
			2016	5
			3016	140
			1017	5
			2017	7
			3017	16
			1018	270
			201A	3
			301A	80
			401A	10
			1109	266
			4109	256
22	TH232	764		
			1001	78
			1009	78
			2009	302
			1003	78
			1014	26
			2014	7
			3014	107
			1016	9
			2016	5
			3016	5
			1017	5
174	U234	1111		
			1001	93
			1009	93
			2009	187
			1003	93
			1004	30
			2004	3
			1006	26
			2006	3
			1007	21
			2007	3
			100A	14
			200A	3
			1009	12
			2009	3
			1010	11
			2010	3
			1014	26
			2014	21
			3014	117
			101A	11
			201A	5
			3016	215
			1017	5
			2017	7
			3017	79
			101A	46
			201A	3
			301A	30
			401A	7
			1109	93
173	U236	1036		
			1001	96
			1009	46
			2009	182
			1003	46
			1004	24
			2004	3
			1006	18
			200A	3
			1007	14
			2007	3
			100A	13
			200A	3
			1009	10
			2009	3
			101A	9
			2010	3
			1014	21
			2014	21
			3014	117
			101A	10
			201A	5
			3016	215
			1017	5
			2017	7
			3017	79
			101A	46
			201A	3
			301A	30
			401A	5

CONTENTS OF GALAXY LIBRARY TAPE FILE NO 3

TOTAL 11863 RECORDS

MFN	MATERIAL	RECORDS	REACTION	RECORDS
228	HE3	195		
			1001	30
			1009	28
			2009	69
			1003	28
			1107	28
			1104	10
221	HE4	230		
			1001	11
			1009	11
			2009	205
214	LI6	593		
			1001	48
			1009	49
			2009	133
			1004	49
			1006	19
			2004	3
			1009	19
			2009	71
			3009	49
			1024	9
			2024	5
			3024	9
			1107	49
			1104	16
			1107	49
215	LI7	496		
			1001	48
			1009	38
			2009	117
			1004	38
			1006	27
			2004	3
			1014	7
			2014	5
			3014	9
			1022	14
			2022	58
			3022	71
			1024	6
			2024	5
			3024	9
			1107	38
			1104	7
254	N	1534		
			1001	510
			1009	510
			2009	197
			1007	510
			1004	82
			2004	3
			1004	26
			2004	3
			1015	66
			2015	3
			3015	13
			1016	11
			2016	5
			3016	25
			1109	510
			1103	510
			1104	66
			1105	82
			1107	194
			1108	17
33	O	1095		
			1001	136
			1009	136
			2009	293
			1003	136
			1004	31
			2004	3
			1005	26
			2005	3
			1006	26
			2006	3
			1007	17
			2007	3
			1008	16
			2008	3
			1004	9
			2009	3
			1010	7
			2010	3
			1011	7
			2011	3
			1012	6
			2012	3
			1013	6
			2013	3
			1014	6
			2014	3
			1015	7
			2015	3
			3015	30
			1109	6
			1103	11
			1104	11
			1107	89
23	F	248		
			1001	41
			1009	41
			2009	37
			1009	41
			1015	25
			2015	3
			3015	37
			1016	5
			2016	5
			3016	5
			1101	41
105	NA	292		
			1001	45
			1009	45
			2009	27
			1009	45
			1015	16
			2015	3
			3015	83
			1016	6
			2016	5
			3016	5
			1101	45
190	TL	681		

235	GD5V	F1
236	WI58	39
237	CU03	F1
208	Y8V	F
238	ZR9Q	12
206	RH1QJ	12
239	IN115	27
240	I127	13
209	TP169	4
210	LU175	9
172	V4L	12
55	17V	15
96	SC4I	12
151	A8J	15

1103	30
1109	69
1014	10
1109	27
1014	10
1109	50
1014	5
1014	10
1014	10
1005	25
101A	11
1014	6
1014	6
1001	3
100P	3
200P	3
1001	3
100P	3
200P	3
110P	
1001	3
100P	3
200P	3
1001	3
100P	3
200P	3
1109	3

CONTENTS OF GALAXY LIBRARY TAPE FILE NO 5

TOTAL 6537 RECORDS

DFN	MATERIAL	RECORDS	REACTION	RECORDS
701	BPM1	88	1107	86
702	SER2	88	1107	86
703	RPB3	80	1107	78
704	RBR4	80	1107	78
705	RBR5	80	1107	78
706	RBR5	80	1107	78
707	RP66	85	1107	83
708	RBB7	83	1107	81
709	SRB8	88	1107	86
710	SMB9	88	1107	96
711	Y89	83	1107	81
712	ZN90	83	1107	81
713	Y90	88	1107	86
714	Y91	98	1107	86
715	ZN91	83	1107	81
716	ZN92	83	1107	81
717	ZR93	88	1107	96
718	ZN94	82	1107	80
719	MO95	80	1107	78
720	ZN96	82	1107	80
721	MO97	80	1107	78
722	MO98	80	1107	78
723	TC99	83	1107	81
724	MO100	80	1107	78
725	RH101	80	1107	78
726	RH102	80	1107	78
727	RH103	80	1107	78
728	RH104	80	1107	78
729	RH105	88	1107	86
730	PB105	80	1107	78
731	PB106	80	1107	78
732	PD107	80	1107	78
733	PD108	80	1107	78
734	AG109	80	1107	78
735	CD111	88	1107	78
736	IN115	80	1107	78
737	SB125	80	1107	78
738	I127	80	1107	78
739	TE128	83	1107	81
740	I129	80	1107	78
741	TE130	83	1107	81
742	I131	86	1107	86
743	XE131	80	1107	78
744	XE132	82	1107	80
745	XE133	98	1107	86
746	CS133	80	1107	78
747	XE134	82	1107	80
748	CS134	88	1107	86
749	I135	88	1107	86
750	XE135	88	1107	86
751	CS135	80	1107	78
752	XE136	83	1107	81
753	CS137	88	1107	86
754	BA138	85	1107	83
755	LA139	87	1107	80
756	CL140	80	1107	78
757	PR141	90	1107	78
758	CE142	87	1107	80
759	ND143	98	1107	86
760	ND144	83	1107	81
761	ND145	83	1107	78
762	ND146	83	1107	81
763	PM147	83		

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P4   P4   P4   P4   P4   P4   P4   P4   P4   P4   P4   P4   P4   P4   P4   P4
1100 1100 1100 1100 1100 1100 1100 1100 1100 1100 1100 1100 1100 1100 1100 1100
0    0    0    0    0    0    0    0    0    0    0    0    0    0    0    0
ND1H6 PqQH8 PeHH4 SqE19 WQ1Hv SmI5G SmI51 SmI6F EmJ5J JmI5K EmI5K EmI5c GmI5b GmI5b GmI57
P64  P65  P66  P67  P68  P69  P70  P71  P72  P73  P74  P75  P76  P77  P78
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